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SIMULATING THE INTERACTION OF ELECTROSTATICALLY CHARGED PARTICLES IN THE INFLOW AREA OF CABIN AIR FILTERS USING A FULLY COUPLED SYSTEM

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Abstract. Precise simulations of particulate flow through fibrous filters are essential in order to predict and enhance filtration performances. To run the computation in reasonable time, a continuum approach is commonly used to emulate the air flow. The software GeoDict [1] allows for the simulation of the complete process, ranging from calculating a flow field, tracking particles inside that field to finding collisions with porous filter media. However, this approach completely neglects particle-particle interactions although particles often carry electrostatic charges [2]. Comparing the results of GeoDict to a fully coupled system shows the influence of this simplification. The software ESPResSo [3, 4] uses such a four-way coupling combining a molecular-dynamics-like approach for partricle simulation with an integrated Lattice-Boltzmann fluid dynamics solver. Already

for a simple scenario, which represents the filter media as a mesh consisting of cylindrical fibers, significant influences of the full coupling on the particle trajectories and even the collection efficiency can be observed. We decribe the modeling and setup for both approaches and present numerical results for simplified yet meaningful test cases.

1 INTRODUCTION

Cabin air filters are applied to prevent small particles such as pollen, fine dust and soot amongst others from being transferred through the HVAC system into the interior (cabin) of a vehicle. Further enhancement of the fibrous filters with regard to filtration efficiency, pressure drop and dust holding capacity is essential due to steadily increasing requirements on air quality in car cabins as well as increasing exposure to pollutants at the same time – especially in fast-growing markets like China. One promising approach to achieve improved filtration performances maintaining a decent differential pressure level is the electrostatic charging of the fibrous media. Thus, electrostatic filtration effects supplement the well-known mechanical collection mechanisms (such as inertia, diffusion, etc.). However, the lack of long-time stability of the charges is a major problem. As traditional development methods are no longer sufficient at this point because they reach their limits of feasability and, moreover, are too expensive virtually prototyping filter media has been an ongoing research subject for years [5]. Regarding the simulation of electrostatic separation mechanisms the fundamentals are still missing. Besides the interference of several fiber-particle interactions (i.e. Coulombic attraction/repulsion, induced dipolar forces, image charge effects) particle-particle interactions potentially play an important role. However, this effect is completely neglected in previous research studies due to the high degree of complexity [2]. In this work, we introduce a new and basic approach to simulate filtration performances using a fully-coupled system. Similarities and differences to the standard one-way coupling approach are presented in detail.

2 ONE-WAY COUPLING APPROACH

In the one-way coupling approach, the fluid is treated as a continuum, i.e., the values for density, temperature and velocity in three spatial dimensions can be calculated at any point in time.

2.1 The One-Way Coupled Model

The underlying mathematical model consists of a system of partial differential equations (PDEs) based on physical conserved quantities. In order to model the behaviour of fluids, mass conversation

$$\nabla u = 0, \tag{1}$$

and momentum conservation

$$\rho(\frac{du}{dt} + (u \cdot \nabla)u) = -\nabla p + \mu \Delta u + f \tag{2}$$

must be ensured. In the equations (1) and (2) u denotes the fluid velocity. The left hand side of the momentum equation with ρ being the density, describes the inertial fluid transport along the flow. The first term on the right hand side describes the acceleration due to a gradient in the pressure p. The diffuse movement resulting from the fluid viscocity μ is considered in the second term. Furthermore, external forces f such as gravitational forces are considered in the momentum equation. The combination of both conservation laws together is well-known as the Navier-Stokes equations. For small Reynolds numbers implying laminar fluid flows the inertial term can be neglected yielding the Stokes equations

$$0 = -\nabla p + \mu \Delta u + f, \quad \nabla u = 0. \tag{3}$$

The disperse multiphase flow is subsequently simulated based on the Euler-Lagrange model, i.e., particle tracking is calculated based on a steady-state flow field by solving the ordinary differential equation

$$\frac{dv}{dt} = \underbrace{\gamma\,(u(x) - v(x))}_{friction} + \underbrace{\frac{QE(x)}{m}}_{electrostatics} + \underbrace{B(t)}_{Brownian\ motion} + \underbrace{f}_{external\ forces}. \tag{4}$$

In the equation of motion, v denotes the particle velocity. The friction γ between particles and fluid flow is modeled in the first term. The subsequent term takes into account the electrostatic interaction of the particle charges Q among the electric field E generated by the filter fibers. The influence of elctrostatic attraction or repulsion respectively depends on the particle mass m. The term $B(t)$ corresponds to the diffusive (Brownian) motion and f again models additional external forces.

In this approach, the particle motion is influenced by the flow field, but there is no interaction between severeral particles and no dependency of the flow field from the particle motion.

2.2 GeoDict

The CFD software GeoDict offers modular tools for the simulation of materials and fluid flows in diverse applications. It was mainly developed for modeling porous media and composite materials. For this purpose, GeoDict offers the possiblity to virtually generate structures as well as to simulate multiphase flow physics in porous media. Thus GeoDict is well suited for filtration procedures, oil and gas transport through digital rocks and electrochemical processes in fuel cell and battery media. In this work, GeoDict is used to calculate the particulate air flow through simplified filter media structures with the

FilterDict [2, 6] module.

Flow Field Calculation. In order to solve the flow equations before, after and inside filter media, GeoDict uses an equidistant voxel mesh discretization. The following three PDE solvers are available to solve the (Navier-) Stokes equations.

- The Explicit Jump (EJ) immersed boundary method can only be used to solve the steady Stokes equation on a regular grid.
- The SIMPLE-FFT is an enhancement of the semi implicit methods for pressure linked equations (SIMPLE) which uses a Fast Fourier transformation (FFT) as a fast solver for the pressure Poisson equation. The solver can be used to aquire a solution of the Stokes as well as the Navier-Stokes equations.
- The LIR (Left Identity Right) solver uses a simplified LIR-tree for spatial partitioning. Thus, it is possible to coarsen the voxel geometry in areas where the velocity or pressure gradient are small. [7]

Due to its short computational runtime and at the same time low memory requirements for porous media only the LIR solver is deployed in this work. After the solver converges the flow field is kept fix and particles are added to the inflow area.

Particle Tracking. During particle tracking, GeoDict permanently searches for collisions of particles with the filter medium. Particles which are captured by the fibers become part of the solid filter structure.

Batch-Wise Geometry Updates. GeoDict uses a batch-wise approach to take into account changes of the filter medium structure due to deposited particles. This means, that we track a batch of (independent) particles along the flow through the filter medium and determine as described above whether or not each particle is captured by a fiber. The batch contains a certain number of particles. After finishing the calculations for the whole batch, the fiber structre is updated, i.e., enhanced by the captured particles. Subsequently, a new flow field is calculated and the next batch of particles is tracked and so forth.

3 FULLY COUPLED APPROACH

The fully coupled approach models interactions between single molecules or particles based on a molecular dynamics like method (MD) and includes the full transient interaction between flow and particles. Therefore, the approach allows for more precise simulations of particle trajectories and becomes suitable for the simulation of particle dynamics in porous filter media.

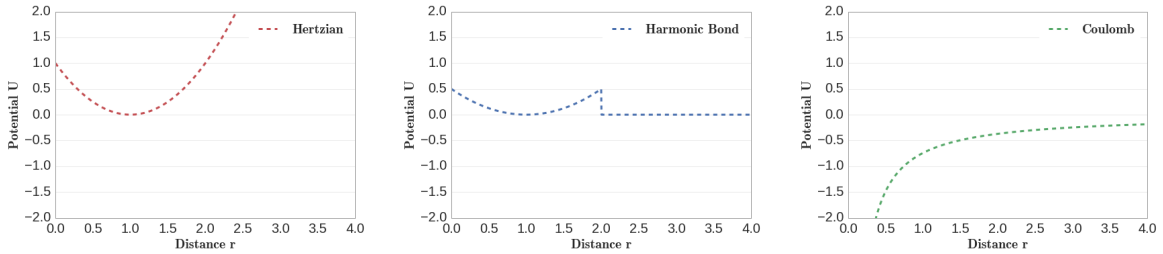

Figure 1: Most important potentials (Hertzian, harmonic bond and Coulomb) regarding interactions in cabin air filtration as a function of the distance between two particles.

3.1 The Fully Coupled Model

The basic component of each particle interaction is the the potential energy $U(|\mathbf{r}|)$ induced by each pair of particles. $U(|\mathbf{r}|)$ depends on the distance $\mathbf{r}$ between two interacting molecules, is described with simple mathematical equations and allows for the calculation of the force $\mathbf{F}(|\mathbf{r}|)$ according to

$$\mathbf{F}(\mathbf{r}) = -\nabla U(|\mathbf{r}|) \quad \text{with} \quad U(|\mathbf{r}|) = U_{Hz}\left(|\mathbf{r}|\right) + U_{hb}\left(|\mathbf{r}|\right) + U_{C}\left(|\mathbf{r}|\right). \tag{5}$$

The equation of motion

$$\ddot{\mathbf{r}} = \frac{\mathbf{F}(\mathbf{r})}{m} \tag{6}$$

describes the resulting particle transport.

For dust particles, we use the Hertzian potential U_{Hz} in combination with two other potentials. The Hertzian potential

$$U_{Hz}\left(|\mathbf{r}|\right) = \epsilon \left(1 - \frac{|\mathbf{r}|}{\sigma}\right)^{\frac{5}{2}}, \tag{7}$$

which is plotted in Fig. 3.1 models collisions of deforming particles [14]. The loss of energy due to deformation ought to be more realistic for the collision of dust particles than the Lennard-Jones potential which is usually used in molecular dynamics for gaseous transport.

The second potential plotted in Fig. 3.1 is implementing dynamic bonding mechanisms. These bond potentials are switched 'on' during the simulation whereever particles collide, thereby friction between the touching particles is assumed. In the simulations of this work a harmonic bond potential

$$U_{hb}\left(|\mathbf{r}|\right) = \frac{1}{2}k\left(|\mathbf{r}| - R\right)^2 \tag{8}$$

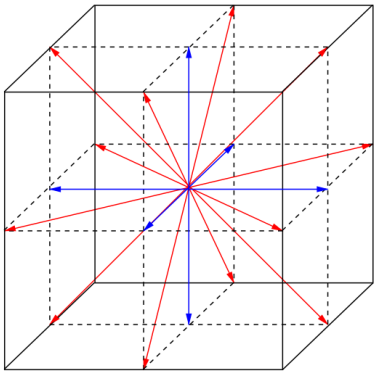

Figure 2: The 19 velocity vectors $\mathbf{c}_i$ for a D3Q19 lattice. From the central grid point, the velocity vectors point towards all 6 nearest neighbours marked in blue and towards 12 next-to-nearest neighbours shown in red. The 19th velocity vector is the rest mode (zero velocity). [15]

is used. The potential is minimal at the distance R and the prefactor is given by k. The described collision detection is especially important when particles carry electrostatic charges. They result in attractive forces which are modeled by the long-ranged electrostatic Coulomb potential

$$U_C\left(|\mathbf{r}|\right) = l_B k_B T \frac{q_1 q_2}{|\mathbf{r}|} \tag{9}$$

that is effective even for large distances. Besides the slow decay for large distances, the Coulomb potential further is singular at $r = 0$.

In addition to the interaction between particles, the fully coupled approach takes into consideration the bi-directional interaction between particles an the backgroud air flow, modeled by the Lattice-Boltzmann method (LBM) approximating the Navier-Stokes equations. LBM is based on mesoscopic kinetic equations. The main idea is that gases or fluids consist of a large number of microscopic particles. During their movement the particles exchange momentum and energy through streaming and particle collision. This particle transport can be modeled with the Boltzmann equation given by

$$\frac{df\left(\mathbf{x}, \mathbf{p}, t\right)}{dt} = \Omega\left(f\right), \tag{10}$$

where $f(\mathbf{x}, \mathbf{p}, t)$ denotes the particle distribution depending on position $\mathbf{x}$, momentum $\mathbf{p}$ and time t. The collison operator (modeling firiction/diffusion) is Ω. To make the equations solvable, LBM discretises the velocity space with a finite number of discrete velocities $\mathbf{c}_i$ and finite differences on a cubic grid in the three-dimensional coordinate space. Fig. 2 shows the widely used D3Q19 discretisation for velocities with 19 velocity components associated to the center of a three-dimensional cubic grid cell. The two algorothmic step of LBM, the streaming (modeling convection) and collision steps can be

calculated according to

$$\underbrace{f_i\left(\mathbf{x}+\mathbf{c_i}dt, t+dt\right) - f_i\left(\mathbf{x},t\right)}_{streaming} = \underbrace{-\frac{dt}{\tau}\left(f_i\left(\mathbf{x},t\right) - f_i^{eq}\left(\mathbf{x},t\right)\right)}_{collision} = \Omega_i. \tag{11}$$

The bi-directional interactions between particles and background flow are considered by the point-coupling between MD and LBM described in [13].

3.2 ESPResSo

The software package ESPResSo (Extensible Simulation Package for RESearch on SOft matter), is based on a molecular dynamics approach for soft matter simulations. Classical examples for soft matter systems are polymers, colloids, liquid crystals or glasses [3]. Besides these applications ESPResSo was originally developed for, the sofware package meanwhile also comprises efficient algorithms for electrostatics [8, 9, 10, 11, 12], dielectrics, magnetostatics and hydrodynamics. By means of coarse-graining ESPResSo enables simulations with diverse length scales on a mesoscopic level. That also allows for yoking molecules together to dust particles in the size of one µm as they occur in real aerosols. Furthermore, the molecular dynamics simulation allows to be coupled to a Lattice-Boltzmann fluid dynamics solver in order to simulate background fluid flows [13]. Therefore, ESPResSo provides a new and basic approach for the simulation of cabin air filtration.

MD in ESPResSo. ESPResSo provides a wide range of interaction potentials [3], among them all potentials required in this work. Regarding the implemented algorithms, a distinction is made between short- and long-ranged interactions. The p3m algorithm of ESPResSo separates the two classes, tackling the short-ranged potential in real space based on cut-off and a linked-cell algorithm, and handling the (smooth) long-range potentials in Fourier space [3].

Lattice-Boltzmann in ESPResSo. In ESPResSo, the fluid particle densities are located on the nodes of the lattice and a linear relaxation towards the equilibrium distribution f_i^{eq} is assumed. Besides the MPI parallized CPU version ESPResSo can also employ GPU acceleration for hydrodynamics [15] which is exploited in this work.

Coupled Simulation in ESPResSo. The fully-coupled model realizes a four-way coupling for simulations of particulate flow through a porous medium. Due to the high degree of complexity, the computational effort is very high, but ESPResSo delivers very precise results for the simulation of particle trajectories.

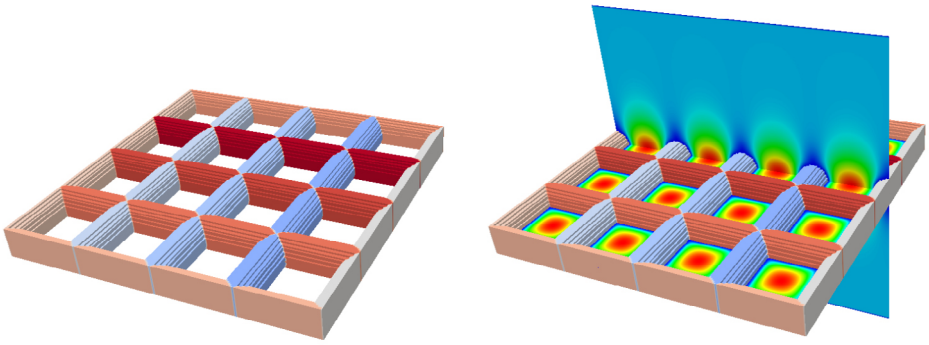

Figure 3: The simulation setup consists of uniformly aligned cylindrical fibers creating a mesh. On the right hand side scliced plots of the magnitude velocity are shown.

4 EXPERIMENTAL SETUP

Since the computational effort becomes immense when considering the fully coupled approach, the experimental setup is chosen as a simple scenario. Fig. 3 shows the used fiber network consisting of uniformly aligned cylindrical constraints. The particulate flow through this mesh is simulated with both software approaches, GeoDict and ESPResSo. The cubic simulation domain has a size of $(200 \times 200 \times 200)\,\mu m^3$ and is assumed to be periodic in each direction for the flow field as well as for the particles. After the flow field has converged, spherical monodisperse particles of the size of two µm are added at the top of the simulation domain. At this point, two different experiments are performed. In a first step, 20 uncharged particles are distributed statistically and added to the flow fields with the same starting positions for each approach. Thereby, the difference in applying uni- and bi-directional interactions between particles and the background flow field is analyzed. As the simulation domain is relativly small, the particle concentration $c_P = 2.8 \cdot 10^{-2}\,{}^{kg}/_{m^3}$ is chosen excessively high in order to have a reasonable number of particles in the simulation domain. In the second experiment, the focus is on the influence of particle-particle interaction during particle motion. For this scenario only two particles are considered, but they carry electrostatic charges q_1 and q_2 that are multiples of the elementary charge $e = 1.602 \cdot 10^{-19}\,C$ ($q_1 = 0.04\,e$ and $q_2 = -0.01\,e$). q_1 and q_2 are unirealisticaly low but allow for stable simulation without further nmerical measures such as time-step restrictions. Important simulation parameters for both experiments are listed in Tab. 1.

5 RESULTS

Flow field simulation. The stand-alone flow field for the used mesh is plotted in Fig. 3. At this point, ESPResSo and GeoDict provide no visible differences regardless of the used solver.

Flow with neutral particles. The particle trajectories of 20 neutral particles in a

Table 1: Simulation parameters for particles, fibers and air flow

fiber diameter	d_F	20	µm
particle diameter	d_P	2	µm
particle density	ρ_P	2650	$^{kg}/_{m^3}$
mean velocity	u_f	0.2	$^{m}/_{s}$
fluid density	ρ_f	1.204	$^{kg}/_{m^3}$
fluid viscosity	η_f	$1.834 \cdot 10^{-5}$	$^{kg}/_{ms}$

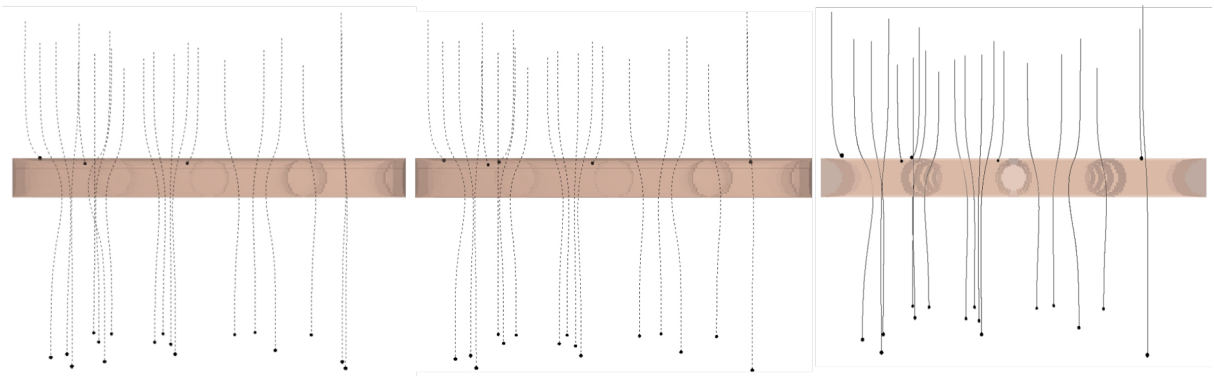

Figure 4: Particle trajectories of 20 particles using the GeoDict Stokes solver, GeoDict Navier-Stokes solver and the ESPResSo LBM for calculating the background air flow.

background flow are plotted in Fig. 4. The two pictures on the left side are both achieved with the LIR solver of GeoDict. The background flow field on the left side is calculated with the Stokes equations whereas the middle one uses the more complex Navier-Stokes equations. The comparison of both GeoDict plots shows minimal deviations in the particle trajectories. However, these deviations result in different collision efficiencies with the fibers. Based on the Stokes flow field, only three particles are captured whereas with the Navier-Stokes version, two more particles stick to the fibers. Already for the small total amount of 20 particles, differences in the collection efficiency can be observed at this point. Tracking the particles with the ESPResSo software package results in the third plot of Fig. 4. Using LBM for the background flow also leads to the deposition of five out of 20 particles. The simulation results point out that for the given flow parameters we are not in the Stokes regime anymore but have to use the Navier-Stokes equations. The comparison between the one-way coupling and the fully coupled approach does not show any effects for this simple scenario.

Flow with charged particles. The simulation results for the two opposite charged particles are displayed in the picture series in Fig. 5. For better viewing, the particles are magnified and their trajectories are additionally plotted again. Although the parti-

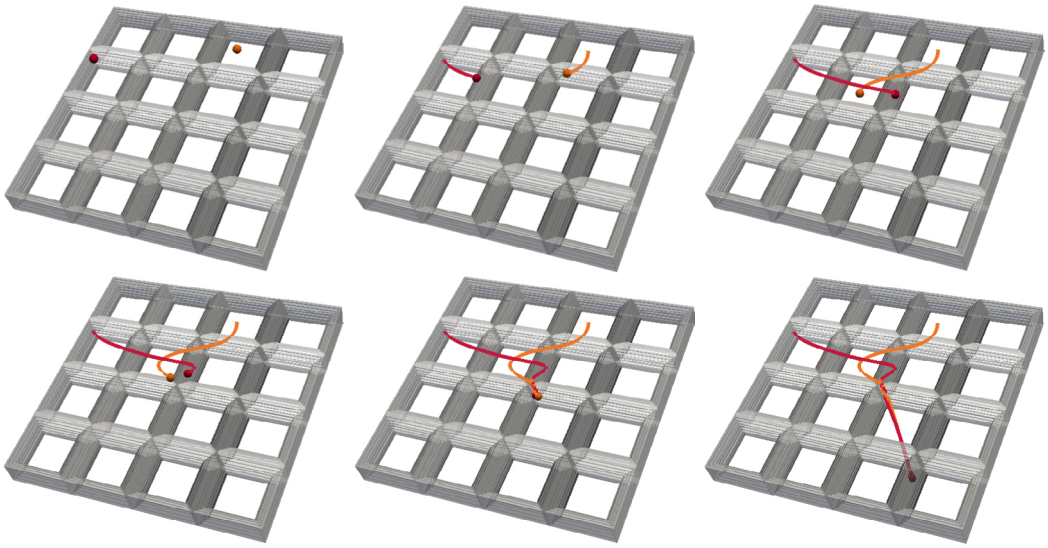

Figure 5: Particle trajectories of two charged particles ($q_1 = 0.04\,e$ and $q_2 = -0.01\,e$) at different times simulated with ESPResSo.

cles only carry extremely low electrostatic charges, we observe a strong attraction and even a collision. The particles already stick together before they reach the fiber network. Subsequently, the particles pass through one of the pores as a kind of agglomerate. The simulation with the same particle starting points is executed without electrostatic interactions. Again a picture series is recorded and plotted in Fig. 6. Omitting the Coulomb potential results in totally different particle trajectories, one particle even collides with the mesh. This points out that particle-particle interactions definitely need to be considered for charged particles.

6 CONCLUSIONS AND OUTLOOK

The preliminary results presented in this paper for particulate air flow through a simple fiber mesh support the assumption that a simple and computationally efficient one-way coupled approach leads to acceptable results as long as we simulate the filtration of uncharged particles in uncharged filter media, only. However, the influence of particles which are added one after the other on the flow field might be more pronounced. Particles thus influence the following particles in the slipstream. As soon as we consider charged particles, already a simulation with only two particles with the fully coupled model shows that particle trajectories change dramatically if particle-particle interactions are properly modeled. The resulting agglomeration of particles into larger clusters is assumed to have an essential effect on filtration efficiency and should therefore not be neglected upon designing filter media exploiting electrostatic effects.

Next steps towards more realistic and application-relevant simulations would be the continous addition of particles (at randomly chose times) instead of at a single point in

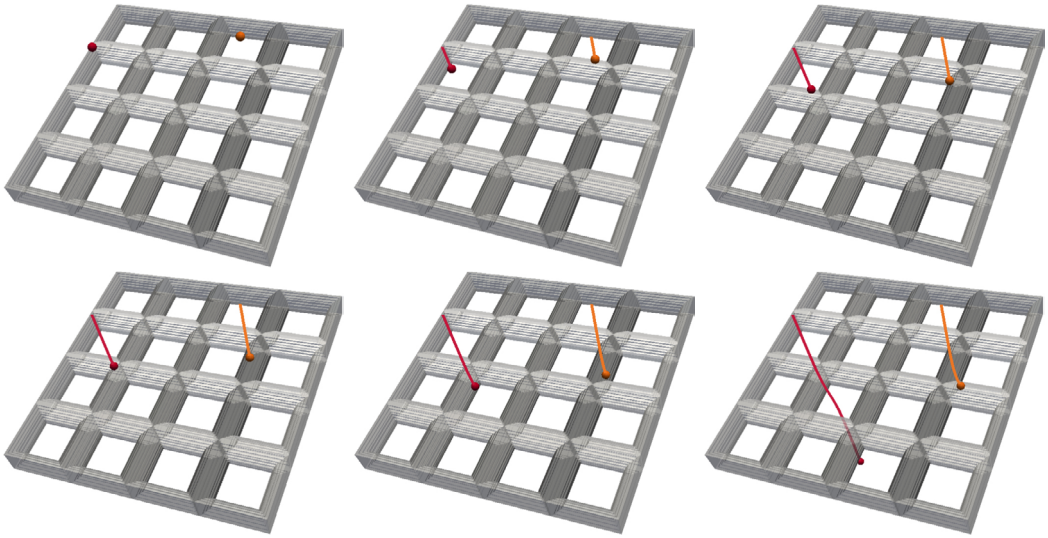

Figure 6: Particke trajectories of two neutral particles at different times simulated with ESPResSo.

time. A new version of the Lattice-Boltzmann solver in ESPResSo working on adaptively refined grids [16] will further allow to simulate more complex filter media structures, larger domain sizes, and longer physical time spans. This enables us to achieve significant simulation results also for lower, more realistic, particle concentrations. Further steps will be the modeling of more realistic charge and particle size distributions and simulations with charged filter media instead of charged particles only.

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